Author(s): Dejun Yang, Tuqiao Zhang, Kefeng Zhang, Duncan J. Greenwood, John P. Hammond and Philip J. White
Article Title: An easily implemented agro-hydrological procedure with dynamic root simulation for water transfer in the crop–soil system: Validation and application
Year of publication: 2009
Link to published version:
http://dx.doi.org/10.1016/j.jhydrol.2009.03.005
Publisher statement: None

An easily implemented agro-hydrological procedure with dynamic root simulation for water transfer in the crop-soil system: validation and application

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No of words in the main body text: 7058

No of figures: 10

No of tables: 6

Abstract

Models for water transfer in the crop-soil system are key components of agro-hydrological models for irrigation, fertilizer and pesticide practices. Many of the hydrological models for water transfer in the crop-soil system are either too approximate due to oversimplified algorithms or employ complex numerical schemes. In this paper we developed a simple and sufficiently accurate algorithm which can be easily adopted in agro-hydrological models for the simulation of water dynamics. We used a dual crop coefficient approach proposed by the FAO for estimating potential evaporation and transpiration, and a dynamic model for calculating relative root length distribution on a daily basis. In a small time step of 0.001 d, we implemented algorithms separately for actual evaporation, root water uptake and soil water content redistribution by decoupling these processes. The Richards equation describing soil water movement was solved using an integration strategy over the soil layers instead of complex numerical schemes. This drastically simplified the procedures of modeling soil water and led to much shorter computer codes. The validity of the proposed model was tested against data from field experiments on two contrasting soils cropped with wheat. Good agreement was achieved between measurement and simulation of soil water content in various depths collected at intervals during crop growth. This indicates that the model is satisfactory in simulating water transfer in the crop-soil system, and therefore can reliably be adopted in agro-hydrological models. Finally we demonstrated how the developed model could be used to study the effect of changes in the environment such as lowering the groundwater table caused by the construction of a motorway on crop transpiration.

Key words: agro-hydrological models, soil water modeling, Integrated Richards Equation (IRE), crop-soil system, plant-soil-atmosphere system.

1. Introduction

The prediction of soil water movement is fundamental to agro-hydrological models for optimizing irrigation, fertilizer and pesticide practices that are so important for the improvement of resource use and the environment. Enormous efforts have been directed to developing models for hydrological simulations in the last few decades (Bastiaanssen et al., 2007).

The hydrological models developed so far in agriculture and horticulture can broadly be classified into two different types. One is a cascade type, and the other is a numerical type based on the Richards equation. In cascade models, soil profiles are divided into a number of layers. Infiltration moves into the soil profile where it is routed through the soil layers. A storage routing flow coefficient is used to predict flow through each soil layer, with flow occurring when a layer exceeds field capacity. Since models of this type are simple and the algorithms are easy to implement without numerical difficulties, many agro-hydrological models have employed this approach for soil water simulation (Arnold et al., 1993; Ritchie, 1998; Greenwood, 2001; Droogers et al., 2001; Brisson et al., 2003; Rahn et al., 2007; Zhang et al., 2007; Renaud et al., 2008). Such models include the prominent CropWat model developed by the FAO which was widely used for irrigation scheduling (http://www.fao.org/nr/water/infores_databases_cropwat.html). However, the determination of the flow coefficient in these models is problematic as the parameter depends on many factors such as the soil water properties, time step and the thickness of soil layer. Therefore, they are often not satisfactory in predicting soil water and are less accurate in estimating evaporation and water uptake by roots. Moreover, it is difficult to implement precisely boundary conditions, such as free drainage, often imposed at the lower boundary in a cascade model, which could result in unacceptable results as the hydrological model is highly sensitive to parameterization at the lower boundary (Boone and Wetcel, 1996).

The numerical model, on the other hand, uses the Richards equation to describe soil water movement. Soil water flow can be simulated accurately in this way provided the soil hydraulic properties are known with certainty. Over the last few decades, substantial progress has been made in this area through advances in mathematics and computer science (Bastiaanssen et al., 2007). The basic theory of water movement in soil is now generally accepted, but the uptake of models of this type is still low (Bastiaanssen et al., 2007). One of reasons for this is the difficulties in making satisfactory estimates of hydraulic properties within soil (Bastiaanssen et al., 2007). There are ways to determine soil hydraulic properties such as direct measurements (Van Genuchten et al., 1991), estimation using pedo-transfer functions (PTFs) (Wösten et al., 1999; Hwang and Powers, 2003; Cresswell et al., 2006), and estimation using inverse modeling techniques (Hopmans and Šimunek, 1999). Progress in predicting soil water retention characteristics based on PTFs has been significant (Cresswell et al., 2006). There was a publication of EU financed work, which provided for the first time the values of hydraulic parameters for a wide range of soils across Europe (Wösten et al., 1999). In the aspect of inferring soil water hydraulic properties using inverse modeling techniques, research has also been active and fruitful (Huyer and Neumaier, 1999; Ines and Droogers, 2002; Jhorar et al., 2002; Ritter et al., 2003; Sonnleitner et al., 2003; Bitterlich et al., 2004; Minasny and Field, 2005; Schmitz et al., 2005). These two lines of evidence suggest that the problem in estimating soil water characteristics has actively been addressed and largely overcome. The other reason that scientists are reluctant to use the Richards equation based models is the complex numerical scheme and the associated long program codes. Since the Richards equation is a highly non-linear differential equation, complex numerical schemes, such as the finite difference method or finite element method, are often employed to solve the equation (Šimunek et al., 1992). This contrasts with the simple algorithms used in modeling other processes such as plant dry matter accumulation, root growth, N mineralization etc. in agro-hydrological models. In addition, these numerical schemes are associated with problems of numerical stability and convergence. It is difficult if not impossible, for un-experienced users to address these problems once they appear.

In order to develop a model which can produce sufficiently accurate solutions and avoids complex numerical schemes, a promising approach named Integrated-Richards-Equation (IRE) model has been proposed (Boone and Wetzel, 1996; Lee and Abriola, 1999). The model considers that water content in a soil layer is only influenced by neighbouring layers, i.e. the above and below layers. The water flux between two soil layers is calculated by integrating the Richards equation over the layer. Thus the whole process of simulating soil water dynamics was drastically simplified and the resulting algorithm was reduced, becoming comparable to that in a cascade model. It has been demonstrated that given a proper time step, the algorithm yielded the same results as these from the finite element solution. However, the work presented by Lee and Abriola (1999) was for water drainage in the soil domain, and did not involve root water uptake and evaporation. Furthermore, the model could not be applied to simulate water flux in the interface between two different soils. Therefore, the proposed model cannot be used directly in agro-hydrological models where both evaporation and root water uptake are the dominant processes in water transfer, and the soil water properties often vary in the profile.

From the above, it is evident that there is a clear need to develop a simple and sufficiently accurate approach to enhance the performance of agro-hydrological models in the simulation of water dynamics, and the IRE based hydrological model has shown its potential to meet this demand. The main purpose of this study was therefore to develop and validate an IRE based hydrological model at a field scale with a dynamic root simulation component as proposed by Pedersen et al. (2007) for water transfer in the crop-soil system. The hydrological model was developed by extending the work of Lee and Abriola (1999) to take consideration of evaporation and root water uptake. Thus the hydrology simulation in agro-hydrological models such as the recently developed model for the combined nitrogen, phosphorus and potassium fertilizers (Zhang et al., 2007), and a major EC financed model for nitrogen fertilizer and irrigation (Rahn et al., 2007), could be updated. Also the study demonstrated how the developed model could be used to study the effects of changes in external environment on water dynamics in the crop-soil system.

2. The model

The model proposed in the study is to provide a simple, approximate but sufficiently accurate, solution to water transfer in the crop-soil system. It works with soil layers with uniform thickness. The thickness of soil layer is fixed as 5 cm which is considered appropriate and commonly used in agro-hydrological models (Greenwood, 2001, Zhang et al., 2007, Renaud et al., 2008) to describe processes such as root length distribution in the crop-soil system. The bottom layer of the calculated soil column is numbered 1, and the soil layer number increases upwards to the top layer. On each day the model first calculates root length distribution, potential daily evaporation and crop transpiration using the FAO dual crop coefficient approach (Allen et al., 1998) based on the measured climatic variables and then implements the following algorithms using a small time step within the day.

- computes the amounts of rainfall, potential evaporation and transpiration for a small step by assuming that all these variables are evenly distributed during a 24 h period;

- calculates the net water influx for the top soil layer by the difference between rainfall and evaporation. If rainfall exceeds potential evaporation, the water flux is treated as infiltration in the top soil layer. Otherwise, the top layer is subject to evaporation;

- assigns the potential transpiration in each of the rooted soil layers, based on the assumption that potential root water uptake is dependent on the root length density;

- computes actual evaporation in the top soil layer and root water uptake in the root occupied layers according to soil water availability;

- applies the IRE algorithm to re-distribute soil water in the simulated domain from layer 1 at the bottom to the top layer. Water movement in the profile can be downwards as well as upwards depending on the soil pressure head in the adjacent layers.

These procedures first on a daily and then a small time step basis are repeated until the end of the simulation period. Detailed formulae of various processes involved in the water transfer are given below.

2.1 IRE algorithm for soil water movement

In 1-D systems, the Richards Equation for water transfer within the soil profile, expressed in terms of soil water content, θ, and soil pressure head, h, is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[K(\theta)(\frac{\partial h}{\partial z} + 1)] \tag{1}$$

The soil hydraulic functions are defined according to van Genuchten (1980) and Mualem (1976)

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = [\frac{1}{1 + |\alpha h|^n}]^m \tag{2}$$

$$K(\theta) = K_s \Theta^{0.5}[1-(1-\Theta^{1/m})^m]^2 \quad (3)$$

where Θ is the relative saturation, θ_s and θ_r ($cm^3\ cm^{-3}$) are the saturated and residual soil water contents, α (cm^{-1}) and n are the shape parameters of the retention and conductivity functions, m=1-1/n, and K_s ($cm\ d^{-1}$) is the saturated hydraulic conductivity.

Eq. (1) is a non-linear differential equation which normally requires complex numerical schemes such as the finite element method to solve it (Šimunek et al., 1992). This involves the procedures of solving a series of linear equations simultaneously in both temporal and spatial domains, resulting in long computer codes which are often associated with the problem of numerical stability. In this study, a simple procedure using an integration strategy of Eq. (1) over the soil layers is employed. The model considers that water content in a soil layer is only influenced by the above and below layers in a small time step, which drastically simplifies the algorithm, allowing soil water flow to be calculated layer by layer. The procedure differs from that by Lee and Abriola (1999) in the form of the Richards equation. Lee and Abriola (1999) used the soil water content based flow equation, which is not applicable to simulate water flow between different soils. This problem is overcome by using the soil pressure head based flow equation as formulated in Eq. (1).

Integrating Eq. (1) vertically over a soil layer leads to

$$\frac{\Delta\overline{\theta_i}}{\Delta t} = \frac{1}{\Delta z}[K_{i+1}(\frac{\Delta h_{i+1,i}}{\Delta z}+1) - K_i(\frac{\Delta h_{i,i-1}}{\Delta z}+1)] \quad (4)$$

where i is the soil layer number, Δt (d) is the time step, $\Delta\overline{\theta_i}$ (cm^3 cm^{-3}) is the layer-average soil water content change in layer i in Δt, Δz (cm) is the soil layer thickness, $\Delta h_{i+1,i}$ (cm) and $\Delta h_{i,i-1}$ (cm) are the differences in soil pressure head between layers i+1 and i, and i and i-1, respectively.

Eq. (4) is an integrated form of the Richards equation for soil water movement. The equation is applied from the layer 1 at the bottom to the top layer for re-distribution of water content in the soil profile at each time step Δt.

2.2 Root growth

There are various approaches in litereture to estimate rooting depth during growth. Greenwood (2001) related the rooting depth with the above gorund crop biomass, while Jiménez-Martínez et al. (2009) assumed that the rooting depth increased with time accoring to a logistic growth function. Experimental evidence shown that root penetration could highly be correlated with the cumulative day temperature over a number of crops (Kage et al., 2000; Kristensen and Thorup-Kristensen, 2004; Thorup-Kristensen, 2006). Based on these findings, a new approach of estimating rooting depth, i.e. daily increment in rooting depth during growth is driven by the mean day temperature, was therefore formulated (Pedersen et al., 2007), and is emplyed in the study. It is recognized though that the used root model is rather simple. It does not account for other factors controlling root growth such as soil water content which can be a limiting factor in dry climates.

$$R_z = R_{z0} + \min\{T_{r\max}, \max[0,(T - T_{base})]\}K_{rz} \qquad (5)$$

where R_z (m) is the rooting depth, R_{z0} is the rooting depth on the previous day, T_{rmax} (^oC) is the temperature for the maximum root growth, T (^oC) is the mean day air temperature, T_{base} (^oC) is the temperature threshold for root growth, K_{rz} (m d^{-1} $°C^{-1}$) is the root growth rate.

The root length declines logarithmically from the soil surface downwards, as originally proposed by Gerwitz and Page (1974). However, contrary to the work of Gerwitz and Page (1974) the rooting depth is extended by 30% from the calculated penetrating depth where the root density declines from a calculated value at the penetrating depth to zero, i.e.

$$L_r(z) = \begin{cases} e^{-a_z z} & z < R_z \\ e^{-a_z z}(1 - \dfrac{z - R_z}{0.3R_z}) & R_z \le z \le 1.3R_z \end{cases} \qquad (6)$$

where L_r(z) is the relative root length distribution, a_z is the shape parameter controlling root distribution down the soil profile.

2.3 Potential soil evaporation and crop transpiration

Vegetation development controls crop transpiration, and also affects soil evaporation resulting from varying cover of ground. It would be ideal that the agro-hydrological models could include the simulation of actual vegetation state such as leaf area index during growth as illustrated in Montaldo and Rondena (2005). However, the models of its kind involve more variants which are crop-specific and some of them are difficult to determine, and thus it is difficult to apply this approach to the agricultural crops where the canopy formation varies vastly. Instead we employed the FAO method (Allen et al., 1998) in the study to estimate water demand for crop growth. The FAO method is not only well parameterized for a wide range of crops, but also has been found one of the most reliable methods to estimate evapotranspiration if the vegetation development does not deviate significantly from that under optimal conditions. In agriculture, crops are normally properly fertilized and irrigated as required, which ensures that the crops grow under sub-optimal conditions. The FAO method has been widely tested over various crops and under different climates, and has been employed in many agro-hydrological models including the most recent ones (Hu et al., 2008; Renaud et al., 2008; Jiménez-Martínez et al., 2009).

Daily potential soil evaporation and crop transpiration are calculated using the dual crop coefficient method proposed by Allen et al. (1998)

$$ET_c = T_{pot} + E_{pot} = (K_{cb} + K_e)ET_0 \qquad (7)$$

where ET_c (mm) is the daily potential evapotranspiration, T_{pot} (mm) and E_{pot} (mm) are the potential daily transpiration and evaporation, respectively, K_{cb}, which depends on crop species and its development stage, is the basal crop coefficient for transpiration (Allen et al., 1998), K_e is the evaporation coefficient, and ET_0 (mm) is the reference evapotranspiration.

ET_0 can be estimated using a Penman-Monteith method directly at daily intervals (Allen et al., 1998)

$$ET_0 = \frac{0.408\delta(R_n - G) + 900\gamma/(T+273)u_2(e_s - e_a)}{\delta + \gamma(1+0.34u_2)} \quad (8)$$

where R_n (MJ m^{-2} d^{-1}) is the net radiation at the crop surface, G (MJ m^{-2} d^{-1}) is the soil heat flux density, u_2 (m s^{-1}) is the 24 h average wind speed at 2 m height, e_s (kPa) is the saturation vapour pressure, e_a (kPa) is the actual vapor pressure, δ (kPa °C^{-1}) is the slope of the vapour pressure curve, and γ (kPa °C^{-1}) is the psychrometric constant.

For the evaporation coefficient, K_e is defined as

$$K_e = \min(K_{c\max} - K_{cb}, fK_{c\max}) \quad (9)$$

where K_{cmax} is the maximum evapotranspiration coefficient, and f is the soil fraction not covered by plants and exposed to evaporation as described by Allen et al. (1998).

2.4 Actual infiltration or soil evaporation

Potential water flux at the soil surface is the difference between rainfall plus irrigation and potential evaporation. The potential water flux is not always met due to the limitation of water contained in the top soil layer or dryness of the soil. In the case of rainfall and irrigation greater than the potential evaporation, the water flux from the surface is considered as infiltration. The actual infiltration flux in a given time step, ΔI_{act} (cm d^{-1}), is determined by the following equation.

$$\Delta I_{act} = \min[(\theta_s - \theta_{Top})\Delta z / \Delta t, w_{Top}] \tag{10}$$

in which, θ_{Top} (cm^3 cm^{-3}) is the water content in the top soil layer, and w_{Top} (cm d^{-1}) is the potential net water flux at the surface.

If the potential evaporation exceeds rainfall and irrigation, the actual evaporation in a given time step from the top soil layer, ΔE_{act} (cm d^{-1}), is expressed as

$$\Delta E_{act} = \min\{K_{Top} \,|\, (h_{\min} - h_{Top}) / \Delta z + 1 \,|, w_{Top}\} \tag{11}$$

where K_{Top} (cm d^{-1}) and h_{Top} (cm) are the soil hydraulic conductivity and soil pressure head in the top layer, respectively, and h_{min} (cm) is the minimum soil pressure head that the atmosphere could possibly exert in the top soil layer.

Under normal field conditions, both soil pressure head and water content at the soil surface are unknown (Aydin et al., 2005), and so is the minimum soil pressure head h_{min}. To estimate h_{min} in the top 5 cm soil layer, we employed a finite element scheme to simulate the distribution of soil pressure head in the region for different soils. The software used was SWMS-2D developed by Šimunek et al. (1992). The calculated soil domain is a column of 1 cm in width by 40 cm in depth, subject to a rapid evaporation of 0.5 cm d^{-1} from its field capacity. Three different soils classified as coarse, medium and fine according to Wösten et al. (1999) were tested. The soil hydraulic properties were adopted from Wösten et al. (1999) and are given in Table 1. The applied minimum soil water potential at the surface was -10^6 cm of water, which was calculated using the Kelvin equation assuming that the water potential at the surface was at equilibrium with the atmosphere (Kirby and Ringross-Voase, 2000; Aydin et al., 2005) and the values of 293 K and 50% for the absolute temperature and the relative air humidity. This value was identical to that set in SWMS-2D for the atmospheric conditions at the soil surface (Šimunek et al., 1992). The model ran for 100 days. At the end of simulation, the averaged soil pressure head over the 5 cm region for coarse, medium and fine soils were -24200, -26100 and -29100 cm of water, respectively. Since these values were close to each other, we simply took the average value of -26500 cm as the minimum water potential h_{min} that the atmosphere could possibly exert in the top 5 cm soil layer, regardless of soil texture. This suggests that the soil water content in the top layer can go below that at the permanent wilting point (h = -15000 cm) caused by evaporation, in line with the recommendation by the FAO that the soil water content can be as low as half soil water content at the permanent wilting point in the evaporative depth (Allen et al., 1998).

2.5 Actual crop transpiration

The actual crop transpiration in a given time step, ΔT_{act} (cm d^{-1}), is the sum of root water uptake from different layers. Following Feddes et al. (1978) and Wu et al. (1999), it is formulated

$$\Delta T_{act} = \Sigma \alpha(h) \Delta S_{\max}(z,h) / \Delta t \tag{12}$$

where α is the root water stress reduction factor, and ΔS_{max} (cm) is the maximum root water uptake in Δt.

It is assumed that all roots have identical physical properties, and therefore have uniform water uptake capacity regardless their age or location. Thus, the maximum root water uptake in Δt can be calculated by assigning the potential transpiration to the root zone

$$\Delta S_{\max}(z) = L_r(z) K_{cb} ET_0 \Delta t / \Sigma L_r(z) \tag{13}$$

The reduction of transpiration caused by the decline in water uptake by the roots in the dry parts of the soil is considered to be similar to that used in Feddes et al. (1978), Šimunek et al. (1992), Wu et al. (1999) and Sonnleitner et al. (2003). Root water uptake is assumed to be zero when soil pressure head is below h_3, i.e. the soil pressure head at the permanent wilting point (h_3 = -15000 cm), and is unlimited for soil pressure head between h_1 (-1 cm) and h_2^{high} (-500 cm) for a rapid transpiration (0.5 cm d^{-1}) and h_2^{low} (-1100 cm) for a slow transpiration (0.1 cm d^{-1}). The increase in water uptake between h_3 and h_2 is linearly related to the soil pressure head. Water uptake is also assumed to be 0 for soil pressure head greater h_1 due to lack of oxygen in the root zone, i. e.

$$\alpha(h) = \begin{cases} 0 & h \le h_3,\ \ h \ge h_1 \\ \dfrac{h - h_3}{h_2 - h_3} & h_3 < h < h_2 \\ 1 & h_2 \le h < h_1 \end{cases} \tag{14}$$

3. Evaluation criteria

The model performance was evaluated using the statistical indices of the coefficient of determination (R^2), the root of the mean squared errors (RMSE) and the mean error (ME) (Bohne and Salzmann, 2002; Ritter et al., 2003; Merdum et al., 2006).

$$R^2 = 1 - \frac{\sum_{i=1}^{N} (Y - Y')^2}{\sum_{i=1}^{N} (Y - \overline{Y'})^2} \qquad (15)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (Y - Y')^2} \qquad (16)$$

$$ME = \frac{1}{N} \sum_{i=1}^{N} (Y - Y') \qquad (17)$$

where Y and Y' are the simulated and measured values, respectively, N is the total number of measurements, and $\overline{Y'}$ is the average of the measured values.

A small RMSE indicates that the simulated values are in good agreement with the measured values. Positive and negative values of ME indicate overall under and over estimation of the predictions.

4. Experiments

4.1 Validation cases

The validation of the model was carried out against data from field experiments with winter wheat conducted at the Institute for Soil Fertility Research, Netherlands from 1983 to 1984 (Groot and Verberne, 1991). The dataset, which was comprehensive including dynamic measurements of soil mineral nitrogen and water contents down the profile, and dry matter accumulations and nitrogen contents in various organs during growth, was widely used for testing fertilizer models at different levels (De Willigen, 1991). The data used in the study was water related only and from two sites with contrasting soils: the Bouwing experiment (silty clay loam) and the PAGV experiment (silty loam). The gravimetrical soil water contents in the layers of 0-20, 20-40, 40-60, 60-80 and 80-100 cm were determined from soil cores taken in 8 replicates at intervals of three weeks from February 1984 in each experiment. The summary of the experiments relevant to the present study is given in Table 2. Details of the experiments can be seen in Groot and Verberne (1991).

4.2 Application case

To demonstrate how the developed model could be used in practice, a numerical investigation of the effect of lowering groundwater table on crop transpiration was carried out. Under the circumstances of high groundwater table, the water supply from groundwater plays an important role to meet crop water demand for growth. Lowering groundwater table restricts water supply from groundwater, and therefore could significantly reduce crop transpiration without proper irrigation. The developed model could be used to estimate irrigation requirement caused by lowering groundwater table to maintain crop yield.

The studied plot is located in Leicestershire, UK (latitude: 52°41'N, longitude: 01°17'W). The monthly mean air temperature and rainfall over the last 20 years are shown in Table 3. The area is one of main vegetable production areas in the UK, and the major crops include Brussels sprouts, potatoes and cabbage. The soil is classified as a sandy loam soil with the topsoil having a depth of 45 cm. A higher percentage of sand and a lower percentage of clay are contained in the subsoil than the topsoil (Table 4). Due to the construction of a motorway, the groundwater table was drastically lowered from about 65 cm to 4 m below the surface before and after the construction. The crop used in the simulations was Brussels sprouts, one of the major crops in the area. Three years' weather data, representing the dry, typical and wet years, respectively, were selected in the study. For each selected year, two scenarios, before the construction (S1), i.e. groundwater table at 65 cm below the soil surface, and after the construction (S2), i.e. groundwater table at 4 m below the soil surface, were run.

5. Model parameterization

5.1 Validation cases

The model parameterization includes the data setting for weather, soil, crop together with initial and boundary conditions. Although the crop was sown in October 1983, no measurements of soil water content down the profile were taken until 07 February, and 14 February 1984 for the Bouwing and the PAGV experiments, respectively. Since the soil water was unknown from the beginning of the experiments to the first measurements, we used the dates of the first measurement of soil water as the starting points in the simulations and set the measured soil water distributions down the profile as the initial conditions. The weather information used in the simulation periods, including daily minimum and maximum air temperatures, rainfall and global radiation, was measured and given in Groot and Verberne (1991).

Soil water retention curves for different layers (0-40 and 40-100 cm) in the Bouwing experiment were obtained from a series of standard curves, while the curves for the PAGV experiment (0-25, 25-40 and 40-100 cm) were measured (Groot and Verberne, 1991). In the study we used van Genuchten functions (Eqs. 2, 3) to describe the soil water retention curves, and the corresponding parameter values were fitted (Table 5) using the RETC software developed by van Genuchten et al. (1991), based on the data provided by Groot and Verberne (1991). Since there were layers of gravel at a depth of about 100-120 cm, which acted as drains, in the Bouwing experiment (Groot and Verberne, 1991), we calculated the soil domain down to 120 cm, and the boundary condition at the bottom was set as free drainage. In the PAGV experiment, the groundwater table was frequently measured and ranged from 86 to 173 cm below the surface. We calculated the soil domain down to 200 cm and set the water content at saturation at the lower boundary. The soil water properties below 100 cm for both cases were taken as the same as those in the layers immediately above.

The crop parameters concerning root growth and root length distribution down the profile were set as follows: the root penetration rate K_{rz} of 0.0007 m d^{-1} ^{o}C^{-1}, the shape parameter controlling root distribution a_z of 3.0, the threshold day temperature for root growth T_{base} of 7 ^oC, the temperature for the maximum root growth T_{rmax} of 27 ^oC. These parameter values were set in line with the study of Rahn et al. (2007). The parameter values used for estimating potential soil evaporation and crop transpiration were according to the FAO dual crop coefficient approach proposed by Allen et al. (1998). The small time step for calculating evaporation, root water uptake and soil water redistribution was 0.001 d as suggested by Lee and Abriola (1999) for 3 cm soil layers.

5.2 Application case

The weather data for the last 20 years (1988-2007) from a nearby weather station which was about 25 km away from the investigated plot was analyzed to determine the dry year, the wet year and the typical year according to yearly rainfall. The year of 1993 was found typical with yearly rainfall of 604 mm, while 1991 and 1999 were found to be the driest and wettest with the yearly rainfall of 462 mm and 770 mm. We, therefore, used the whole year weather data of 1991, 1993 and 1999 for the simulations (Fig. 1). The soil water characteristics were determined using a PTFs approach proposed by Wösten et al (1999), based on the measured soil particle distributions and an assumed bulk density of 1.4 g cm^3 for the sandy loam soil. We considered the proposed functions for estimating soil water characteristics were particularly suitable for the case, as the published work was specifically targeting the European soils. Table 4 shows the soil water characteristics derived using the PTFs approach for the topsoil and subsoil. The planting and harvest dates were 1 April and 1 October, respectively. Since roots do not grow into the saturated soil and cannot take up water from a saturated zone due to lack of oxygen, we considered for scenario S1, i.e. before the motorway construction, the maximum rooting depth was restricted to 65 cm, the average groundwater table. The upper boundary was subject to atmospheric conditions in all the simulations. The soil water content was at its saturation below 65 cm throughout for S1 and free drainage condition was set at the lower boundary (2 m below the surface) for S2 as the groundwater table was far below 2 m (estimated 4 to 5 m). The model ran from 1 January when the soil water content was at its field capacity.

The crop parameters for root growth and root length distribution down the profile, and the small time step for calculating evaporation, root water uptake and soil water redistribution were set the same as those in the validation cases. In the very early crop development stage, the model assumed a constant rooting depth of 0.2 m for the cumulative effective day degree less than 100 d ^{o}C. The parameter values used for estimating potential soil evaporation and crop transpiration were determined according to Allen et al. (1998).

6. Results and discussion

6.1. Model Validation

6.1.1. Model overall performance

To evaluate the overall performance of the model, all the measurements collected from both experiments for validation in the aspects of root development and soil water content in different soil layers were compared with the simulations (Fig. 2). Simulated values of relative root density down the profile at intervals for both the Bouwing and the PAGV experiments were not only highly correlated but almost proportional to the measured values (Fig. 2a). Both RMSE and ME were small, only 0.1258 and 0.0016, respectively (Table 6). This indicates that the model gave good predictions of root dynamics during crop growth. The simulated values of soil water content also agreed well with the measured values (Fig. 2b). Regression of simulated and measured gave a high R^2 of 0.801. And again the values of RMSE (0.0412 cm^3 cm^{-3}) and ME (0.0260 cm^3 cm^{-3}) were small. Over the 99 comparisons only 22 differed by more than 0.05 cm^3 cm^{-3} and 2 by more than 0.1 cm^3 cm^{-3}. The overall agreement between measurement and simulation for both relative root length distribution and soil water content in various layers was good. This suggests that the model performed reasonably well in predicting root and water dynamics in the crop-soil system. Thus the proposed model using relatively simple algorithms has the potential to be adopted in the agro-hydrological models for irrigation, fertilizer and pesticide practices.

6.1.2. Rooting depth and relative root length distribution

Relative root distributions down the soil profile at intervals were simulated and compared with the measurements (Fig. 3). Generally, the model was satisfactory in modeling root dynamics since the agreement between the simulated and measured relative root distributions was good, indicating that the proposed equations describing root growth and parameterization were appropriate for wheat. The difference in the measured relative root distribution between the BOWU and the PAGV experiments might be attributed to the fact the crop grew on different soil textures. Such results could not be reproduced by the model in the study since the model did not consider the effect of soil texture on root growth. The comparison also reveals that the model performed better in predicting relative root length distribution for the crop in the early development stages. The measured root length distribution was well simulated on 25 April, 1984 (Fig. 3a), while the simulated root distributions at later dates deviated from the measurements (Fig. 3bc). In the top 10 cm soil layer the model underestimated the relative root length, whereas the opposite was found to be the case in the 10 – 60 cm soil region. The probable reasons for the difference might be due to the fact that soil water content was not considered in the simulation of root growth, or that the relative root length distribution is dependent on crop development stage, and thus underlines the possibility to further improve the root model in the future.

Comparison of the simulated wheat relative root length distribution in the study with these calculated using available equations (Wu et al., 1999; Zuo et al., 2004) were also carried out (Fig. 4). Zuo et al. (2004) described the root length distribution with a highly non-linear equation with four parameters, while Wu et al. (1999) formulated the distribution with a third-order polynomial equation. It was found that the modeled relative root length distribution in the study was in good agreement with these calculated by Wu et al. (1999) and Zuo et al. (2004) (Fig. 4). In the top and bottom 20% rooting depth the modeled root length distribution in the study was in between those calculated by the equations proposed by Wu et al. (1999) and Zuo et al. (2004), whereas in the middle 60% rooted region, our prediction was close to that by Zuo et al. (2004). Both equations derived by Wu et al. (1999) and Zuo et al. (2004) were based on comprehensive datasets made up from measurements. This indicates that the simple approach used in the study for root dynamics is able to describe root length distribution in the soil for wheat. This, together with the ability of modeling rooting depth, makes the algorithm for root growth reliable for modeling water and nutrient dynamics in wheat-soil systems.

6.1.3. Soil water content in various layers

Soil water contents in 20 cm layers to 1 m were generally well simulated over time for both experiments (Fig. 5). The model not only reproduced the patterns of soil water changes in layers, but also produced values close to the measurements. In the top 20 cm layer, soil water content was markedly affected by rainfall. The peaks of soil water were all coincided with big rainfall events. In the 20-40 cm layer soil water content was less affected by rainfall. There was only one noticeable soil water increase in this layer between Day 142 to Day 184 when big rainfall events concentrated. In the soil layers below 40 cm, rainfall had virtually no direct influence on soil water content. Soil water in these layers decreased constantly due to root water uptake. Despite good overall agreement of soil water content between measurement and simulation, the discrepancies between measured and simulated values were more evident in the 20-40 cm soil layer in the Bouwing experiment and in the top 20 cm soil layer in the PAGV experiment. One possible reason for these discrepancies is inaccurate soil water properties used in the simulation for these two soil layers. The measured or derived soil water properties based on certain approaches might not be representative for the soil at a field scale. Such a phenomenon has been encountered often and reported previously (Hopmans and Šimunek, 1999; Ritter et al., 2003).

6.1.4. Soil evaporation and crop transpiration

High potential soil evaporation occurred before Day 140 and after Day 205 when the crop was at its early development stages and at its late development stage (Fig. 6). In these stages the ground cover was less intense and therefore the evaporation demand was larger. There were two periods from Day 110 to 138 and after Day 205 when the actual evaporation was far less than the potential for the most days. This can be explained by sparse rainfall during these periods and the resulting low soil water content close to the permanent wilting point in the top 5 cm layer (Fig. 7) in both experiments. In the rest growing period soil evaporation was basically met in both experiments. This is because the soils in the top 5 cm layer in these periods were relatively wet in both experiments (Fig. 7).

Contrary to soil evaporation, the biggest crop transpiration demand happened during Day 140 to Day 205 when the crop was at its mid-season development stage (Fig. 8). Wheat grown in the Bouwing experiment suffered from water stress as the cumulative actual transpiration was clearly less than the potential one, while the crop in the PAGV experiment was basically free from water stress (Fig. 8). The cumulative potential transpirations for the Bouwing and the PVGA experiments were 419 and 425 mm, respectively, similar to each other. At the end of the simulation the crop in the Bouwing experiment was only able to extract 257 mm water from the soil, whereas the corresponding value for the PAGV experiment was 383 mm. In the Bouwing experiment water stress occurred mainly in two periods, i.e. Day 108 to Day 145 and after Day 205 when the potential transpiration clearly exceeded the actual one (Fig. 8a), resulting from low water content in the top 20 cm and 20-40 cm layers (Fig. 5) where the most roots located. However, water stress in the PAGV experiment happened only in a brief period between Day 115 to Day 138. This contrasting difference between two experiments was primarily caused by a free drainage in the 100-120 cm layer in the Bouwing experiment, which made the soil water flow upwards impossible from below 120 cm, and the relatively high groundwater table in the PAGV experiment, which made more water available for roots to take up in the lower soil region due to capillary flow.

It should be pointed out that due to the small time step employed in calculating soil evaporation, crop transpiration and soil water movement, the model is flexible to use the weather information collected at shorter intervals, say hourly, to produce more accurate results. The disadvantage is that it takes longer to run the model compared to other approaches. However the computation effort is quite affordable with modern computing equipment. For the cases above it only took a personal PC with a pentium IV processor about 35 seconds CPU time to run each case.

6.2. Model application

The potential and actual cumulative crop transpirations over the growing period from 1 April to 1 October in the dry, the typical and the wet years were simulated for the application case with Brussels sprouts (Fig. 9). The calculated potential cumulative transpiration during growth was 430 mm in the typical year, similar with the values of 441 mm and 420 mm for the dry year and the wet year. The simulations for Scenario S1 in all three different years, i.e. before the motorway construction, show that the crop was basically able to extract water from the soil to meet potential transpiration without irrigation (Fig. 9). However, a significant drop in water uptake was simulated due to lowering the groundwater table resulting from the motorway construction. Without irrigation, the crop was only capable of taking up about 160 mm from the soil in the typical year. Likewise the values are 130 mm and 200 mm for the dry year and the wet year, respectively. The reduction in transpiration was caused by the lack of water supply from groundwater. Simulations reveal there was no upwards capillary water flow at the depth of 50 cm from the surface in S2, whilst a substantial water supply at this depth from groundwater was simulated in S1, and the supply tended to increase with time despite the fluctuations (Fig. 10). The variations of soil water content in different soil layers for both scenarios were also simulated (data not shown). In the top 0-30 cm soil layers, the water content was heavily influenced by rainfall as found in the validation cases. It appears that the influence was limited in the top 30 cm region, since the changes in water content in the soil below was not correlated with rainfall. Also it is clear that the water content in different soil layers in S2 was constantly lower than that in S1 during the growing period.

From the above it can be concluded that the construction of a motorway has a serious negative effect on the ability of a crop to take up water from the soil without irrigation. Since crop transpiration is positively related to the crop yield (Wild, 1988; Allen et al., 1998), the significant reduction in transpiration will inevitably lead to a reduction in yield.

7. Conclusions

An easy-to-use procedure, using an integrated Richards equation solution for soil water movement for water transfer in the crop-soil system, has been derived. Due to the small time step employed in the model, the coupled processes of soil evaporation, crop transpiration and soil water movement were successfully decoupled, leading to simple algorithms that are easily implemented. Thus the complex numerical schemes and associated long program codes for accurate simulation of water dynamics in the crop-soil system are avoided, which makes it easier to use the basic theory of soil water flow in the agro-hydrological models. Further, the small time step makes it possible to use the weather information collected at any time intervals. The validation of the model against data from field experiments on two contrasting soils cropped with wheat showed that the model was capable of making good predictions of soil water content at different depths and at intervals during crop growth. This proves that the proposed algorithms for modeling water dynamics in various processes in the crop-soil system were reasonable and the model was adequately constructed. Since the model is simple and sufficiently accurate for the simulations at a field scale, it has the potential to be employed in agro-hydrological models for irrigation, fertilizer and pesticide practices.

Finally it is worth pointing out that the model developed in the study is a deterministic one which works well when all the input parameters are known with certainty. To further extend the model for prediction purposes, consideration of dealing with parameters with stochastic nature such as rainfall should be made in the future (Laio, 2006).

Acknowledgements

The work was partly financed by the UK Department for Environment, Food and Rural Affairs through the project HH3507SFV. The authors gratefully thank Dr J Neeteson for kindly providing the essential dataset for validating the model proposed in the study. D Yang acknowledges the financial support from the China Scholarship Council for his joint PhD program between Zhejiang University, China, and Warwick University, UK.

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Figure captions:

Figure 1: Rainfall and radiation distributions used in the simulations for the dry year (a), the typical year (b) and the wet year (c) in the application case.

Figure 2: Overall comparison of relative root density distribution at interval (a) and soil water content in various soil layers (b) between measurement and simulation for the Bouwing and the PAGV experiments.

Figure 3: Comparison of relative root distribution between measurement and simulation at intervals of the Bouwing and the PAGV experiments.

Figure 4: Comparison of distribution of normalised root length density proposed in the study with these calculated from literature for wheat.

Figure 5: Comparison between the measured and simulated volumetric soil water content at different soil layers for the Bouwing experiment (a) and the PAGV experiment (b).

Figure 6: Daily and cumulative potential and actual evaporation for the Bouwing experiment (a) and the PAGV experiment.

Figure 7: Variations of soil water content in the top 5 cm soil layer for both the Bouwing and the PAGV experiments (The water contents at the permanent

wilting point in the top 5 cm soil layer for the Bouwing and PAGV experiments are 0.169 and 0.114 $cm^3 cm^{-3}$, respectively).

Figure 8: Daily and cumulative potential and actual transpiration for the Bouwing experiment (a) for the PAGV experiment (b).

Figure 9: Simulated potential and actual cumulative transpiration during growth for scenarios of S1 (before construction) and S2 (after construction) in the dry year (a), the typical year (b) and the wet year (c).

Figure 10: Simulated upwards water flux at 50 cm below the soil surface during growth for scenarios of S1 (before motorway construction) and S2 (after motorway construction) in the dry year, the typical year and the wet year.

Table captions:

Table 1: van Genuchten parameter values in Eqs. (2) and (3) for coarse, medium and fine soils (Wösten et al., 1999)

Table 2: Summary of the Bouwing and the PAGV experiments

Table 3: Monthly average rainfall and mean air temperature in the application case

Table 4: Measured particle size distribution and soil organic matter, and soil hydraulic properties derived using PTFs proposed by Wösten et al. (1999) for the topsoil (0 – 45 cm) and subsoil (45 – 100 cm) in the application case

Table 5: Fitted van Genuchten parameter values in Eq. (12) for the Bouwing and the PAGV experiments using the RETC software (van Genuchten et al., 1991)

Table 6: Statistical comparisons between measurement and simulation of relative root length distribution and soil water content in various layers for both the Bouwing and the PAGV experiments

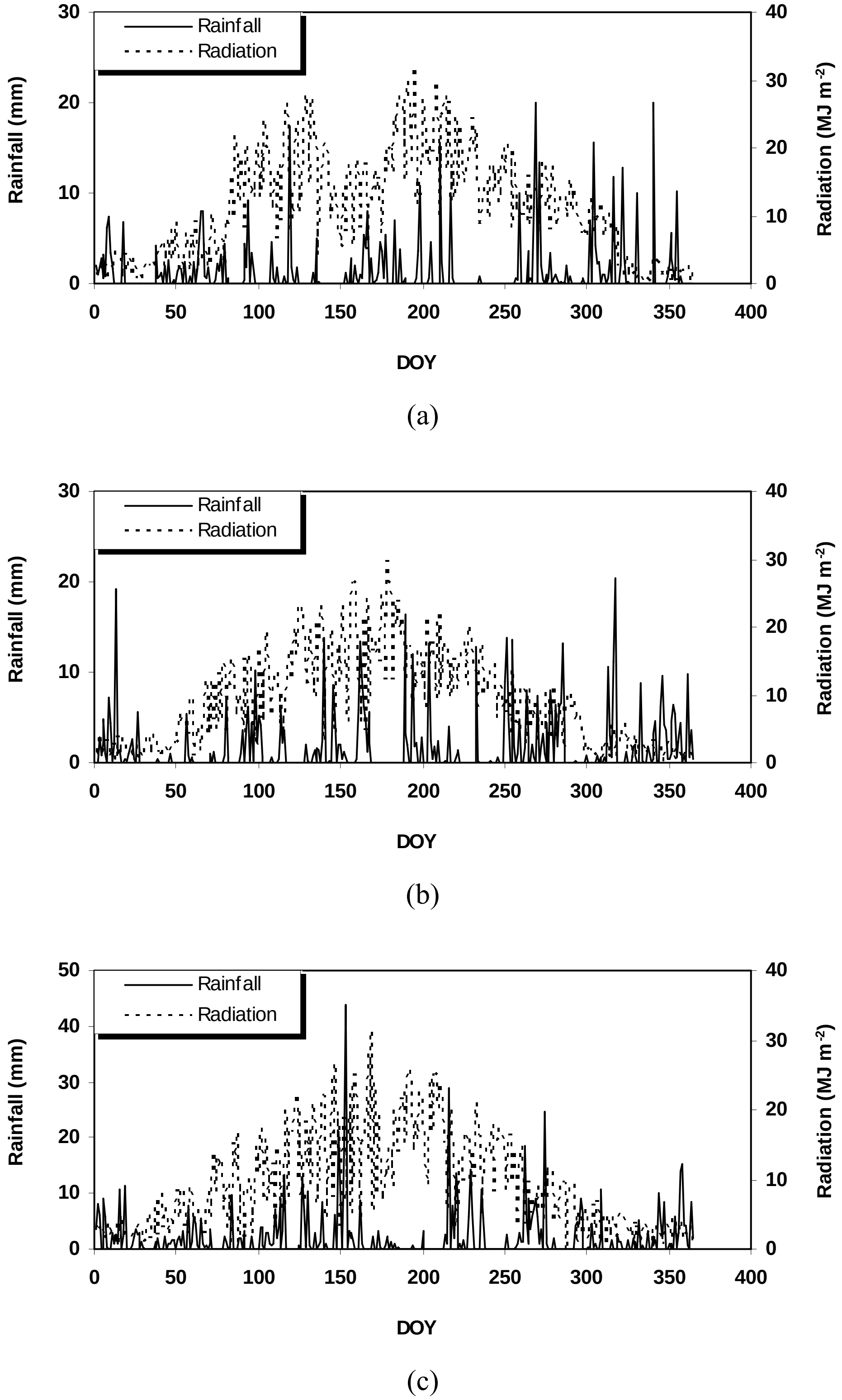
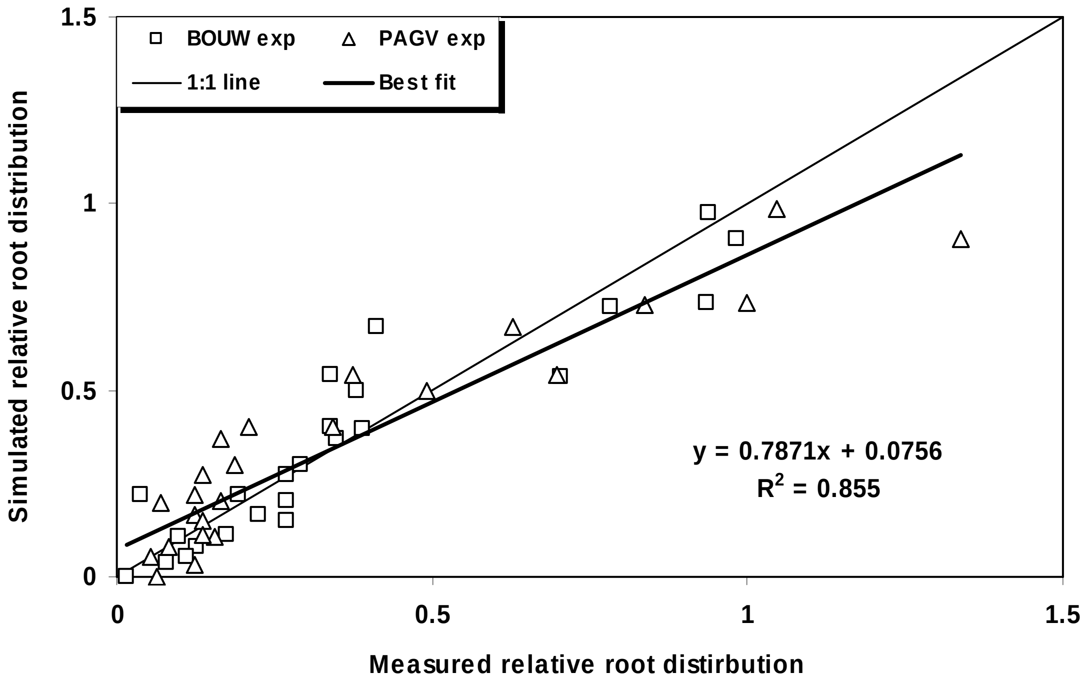
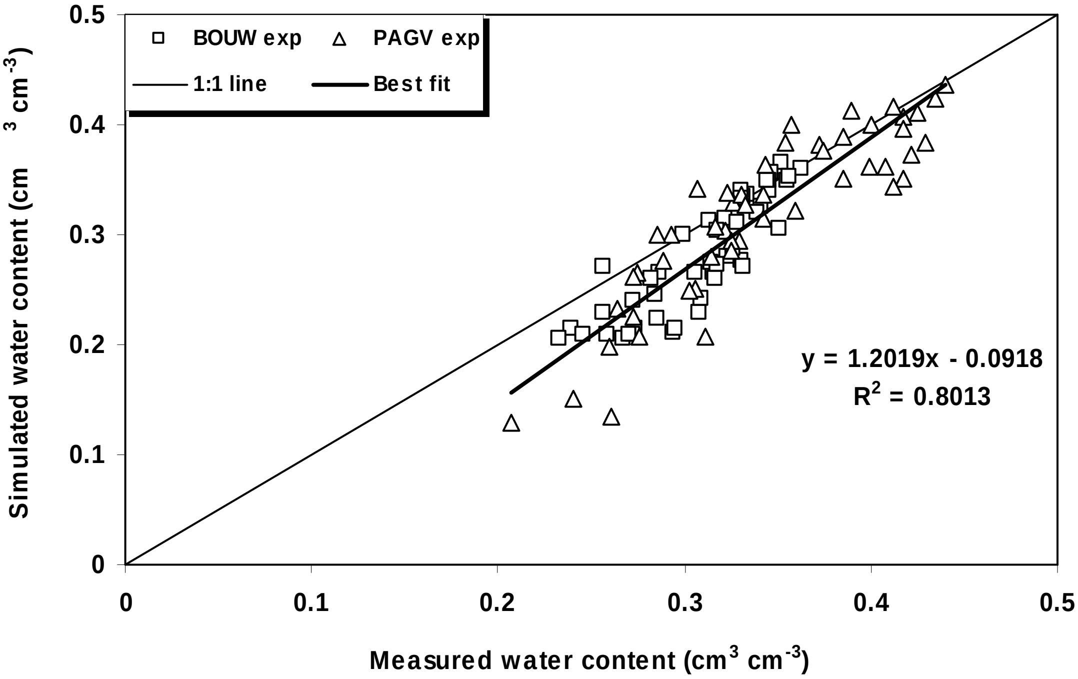

Rainfall
Radiation
Rainfall (mm)
Radiation (MJ m-2)
DOY
0
50
100
150
200
250
300
350
400
(a)
(b)
(c)

Fig. 1

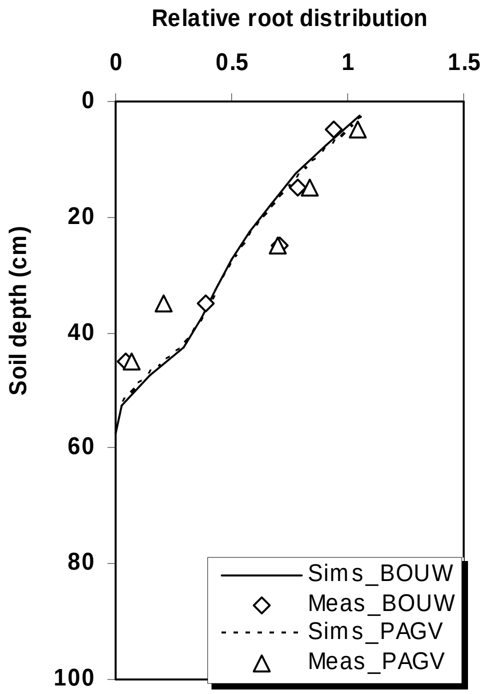

BOUW exp
PAGV exp
1:1 line
Best fit
y = 0.7871x + 0.0756
R2 = 0.855
Simulated relative root distribution
Measured relative root distirbution
0
0.5
1
1.5

(a)

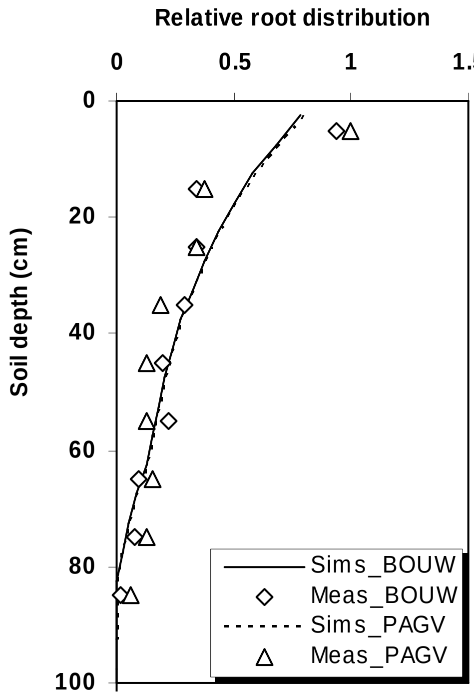

BOUW exp
PAGV exp
1:1 line
Best fit
y = 1.2019x - 0.0918
R2 = 0.8013
Simulated water content (cm 3 cm -3)
Measured water content (cm3 cm-3)
0
0.1
0.2
0.3
0.4
0.5

(b)

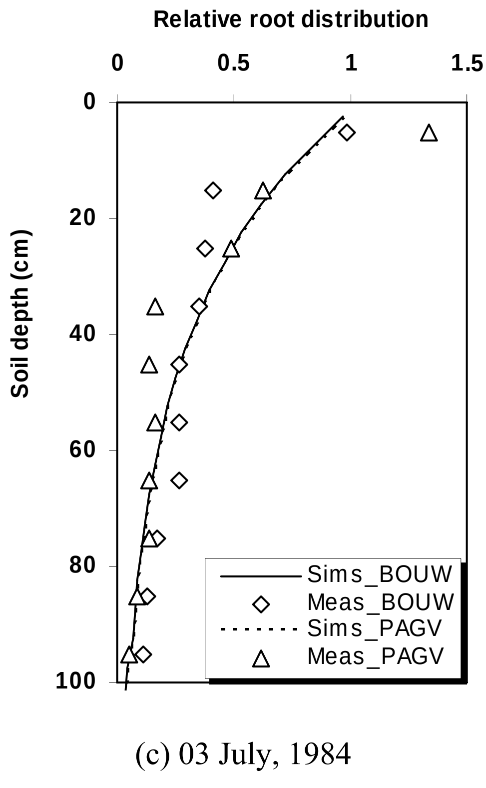
Fig. 2



(a) 25 April, 1984



(b) 05 May, 1984



(c) 03 July, 1984

Fig. 3

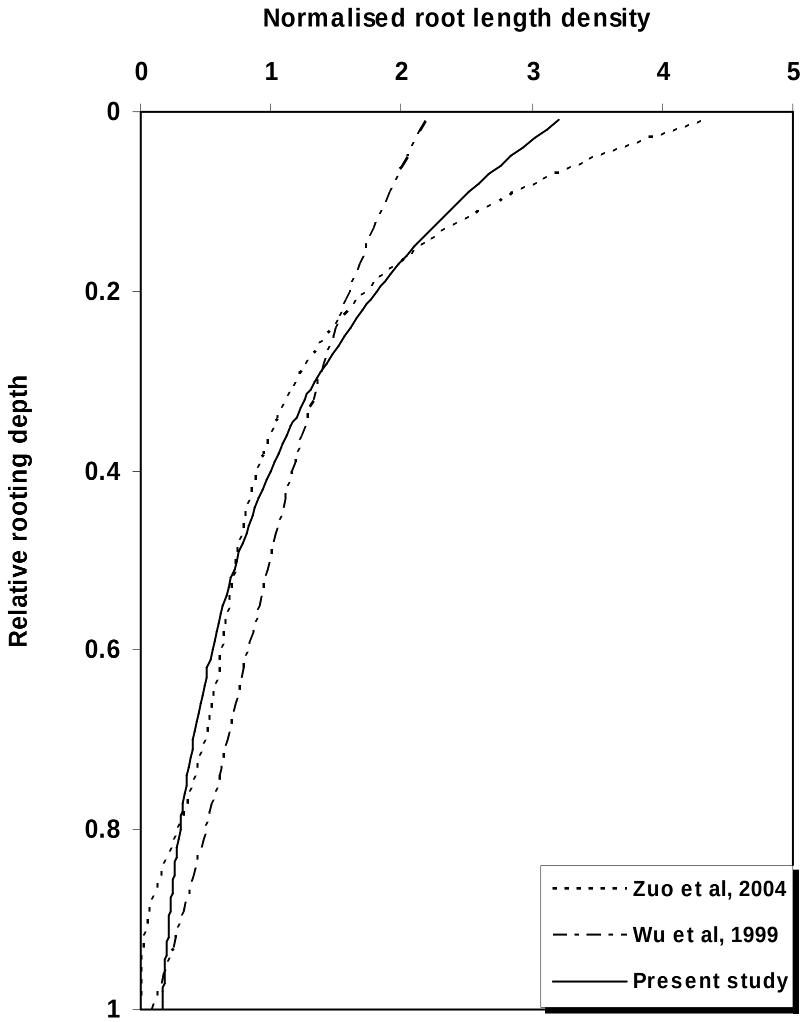
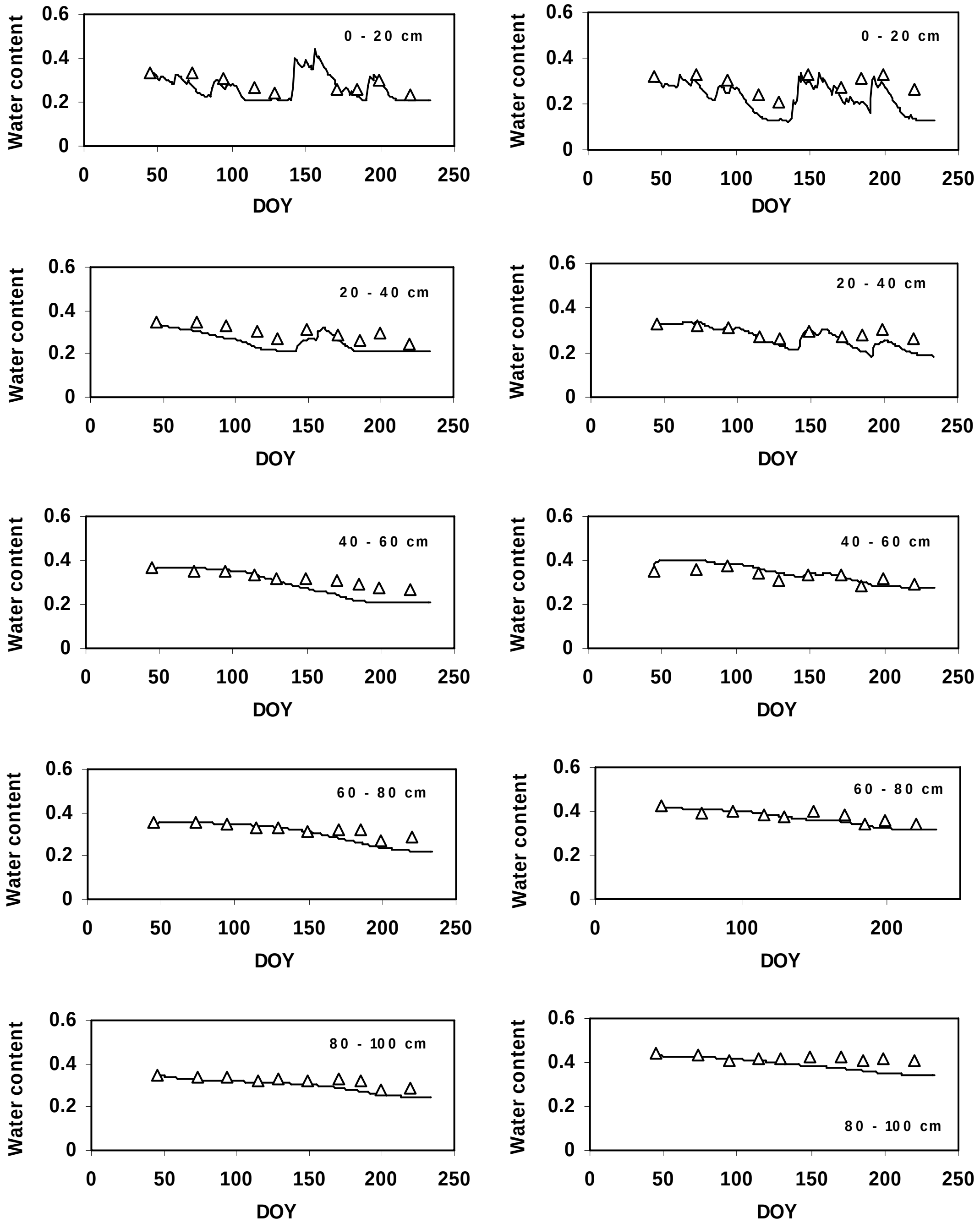
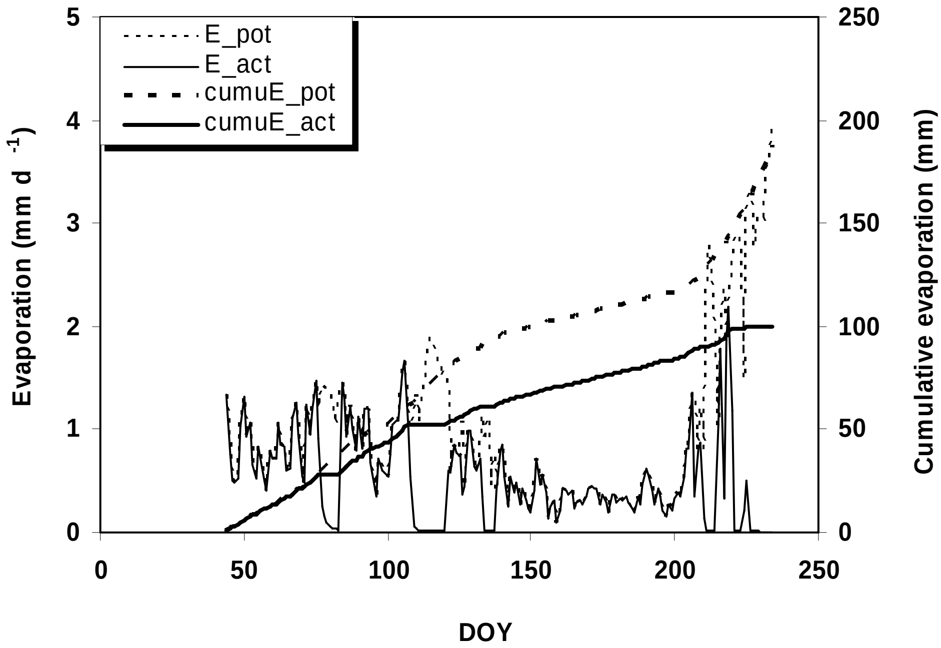

Normalised root length density
0
1
2
3
4
5
0
0.2
0.4
0.6
0.8
1
Relative rooting depth
Zuo et al, 2004
Wu et al, 1999
Present study

Fig. 4

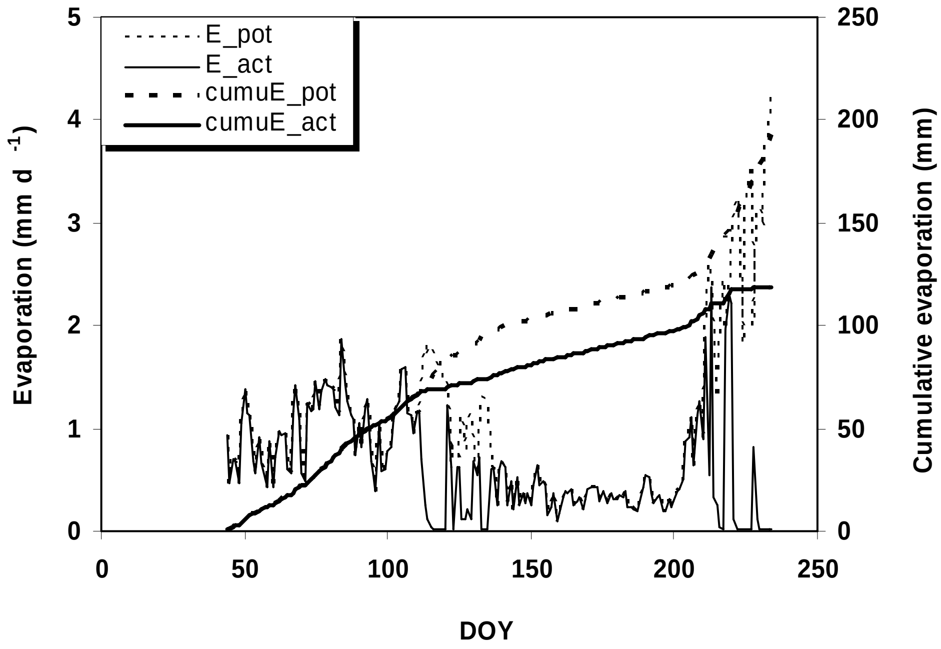


(a) Bouwing (b) PAGV

Fig. 5

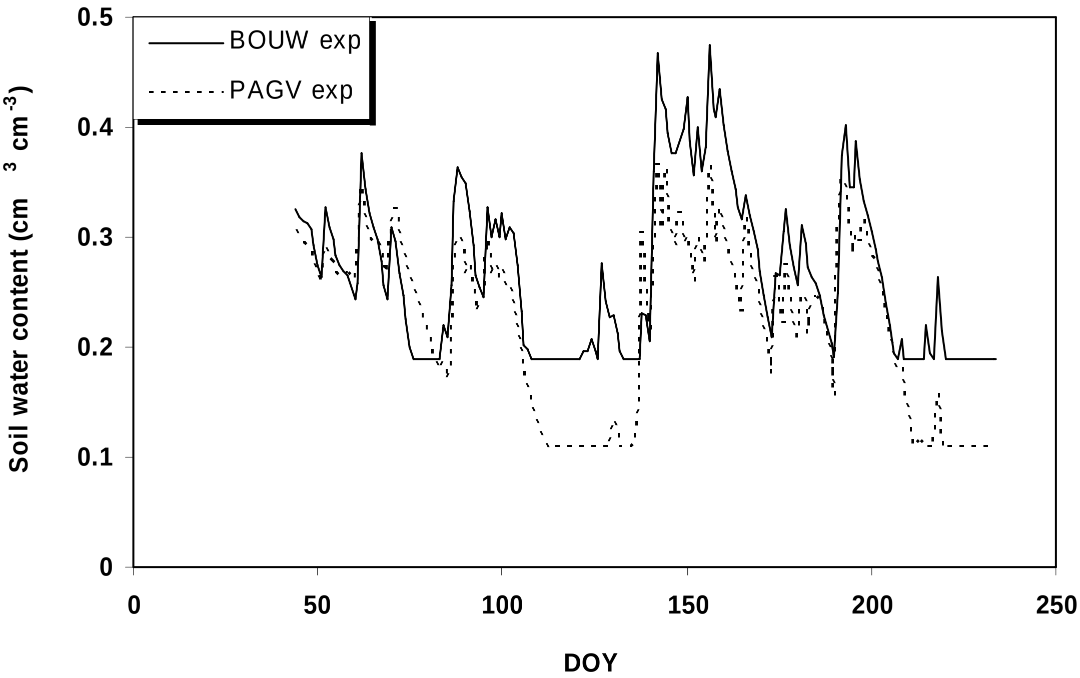

E_pot
E_act
cumuE_pot
cumuE_act
Evaporation (mm d -1)
Cumulative evaporation (mm)
DOY
0
1
2
3
4
5
0
50
100
150
200
250

(a)


E_pot
E_act
cumuE_pot
cumuE_act
Evaporation (mm d -1)
Cumulative evaporation (mm)
DOY
0
1
2
3
4
5
0
50
100
150
200
250

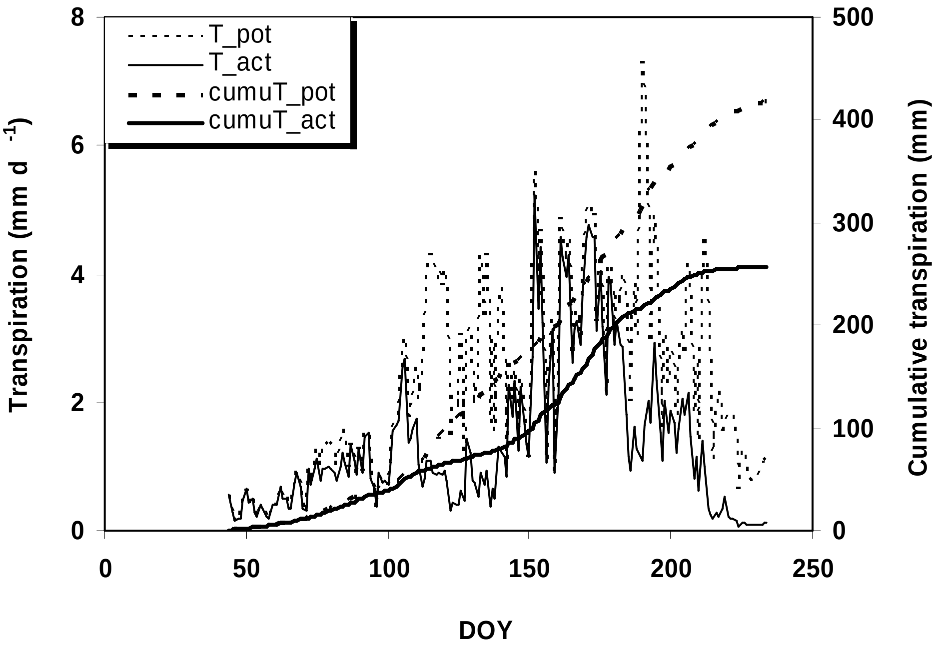
(b)

Fig. 6

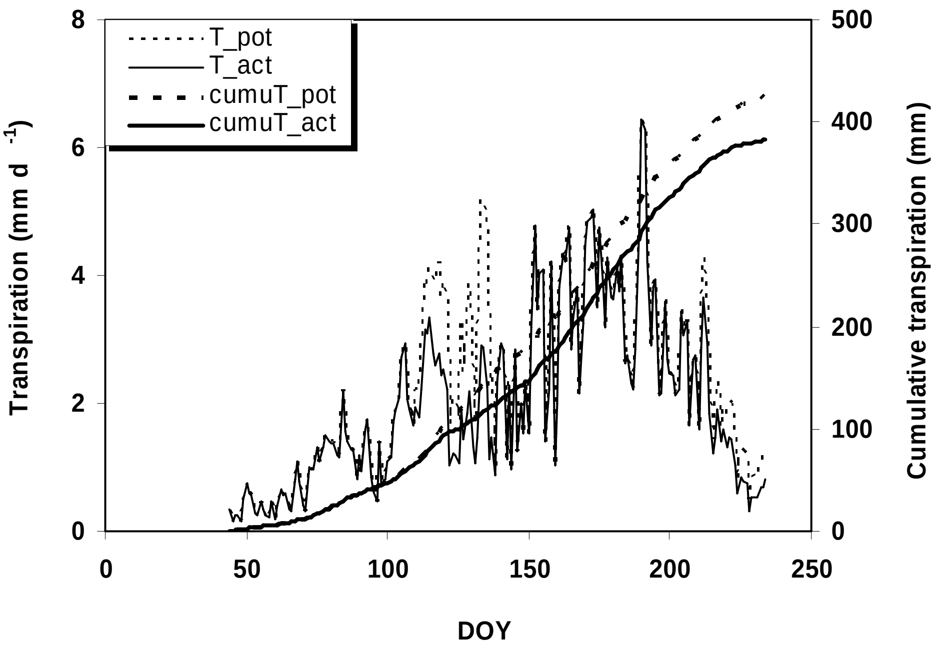


BOUW exp
PAGV exp
Soil water content (cm 3 cm -3)
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
250
DOY

Fig. 7

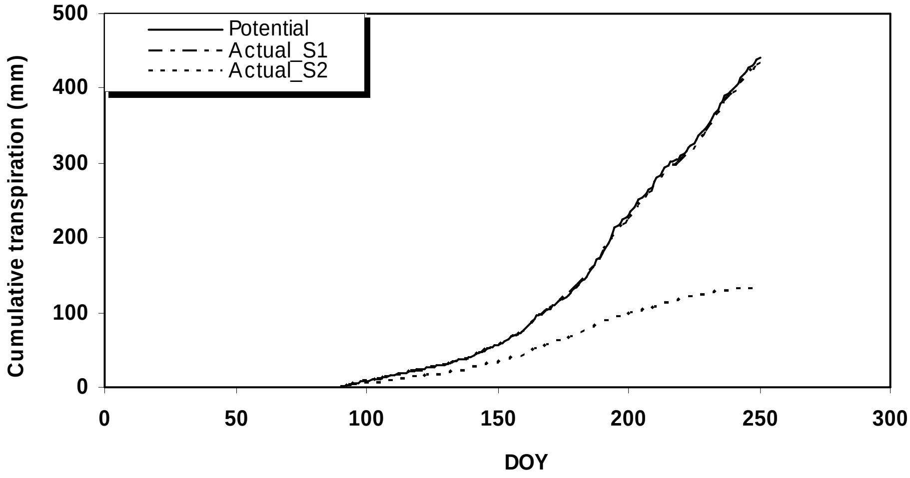

T_pot
T_act
cumuT_pot
cumuT_act
Transpiration (mm d -1)
Cumulative transpiration (mm)
DOY
0
2
4
6
8
0
100
200
300
400
500
0
50
100
150
200
250

(a)

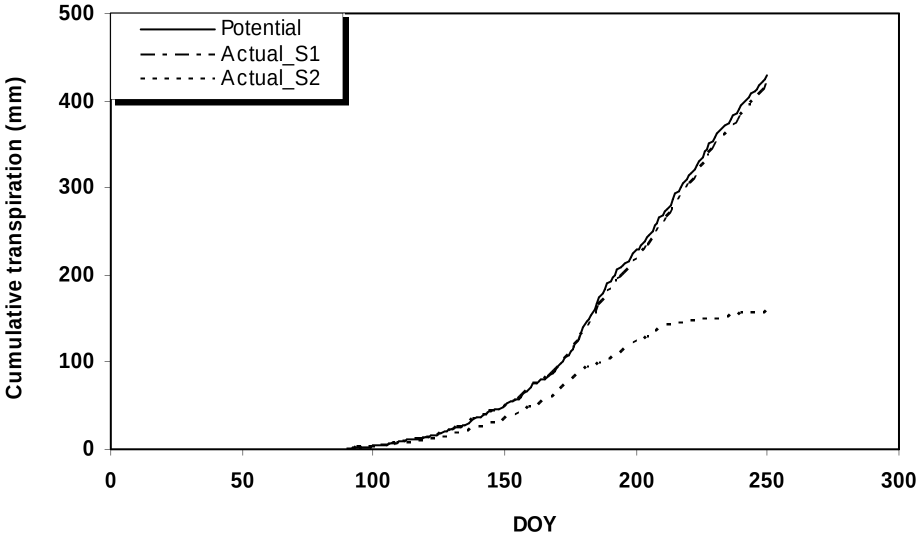

T_pot
T_act
cumuT_pot
cumuT_act
Transpiration (mm d -1)
Cumulative transpiration (mm)
DOY
0
2
4
6
8
0
100
200
300
400
500
0
50
100
150
200
250

(b)

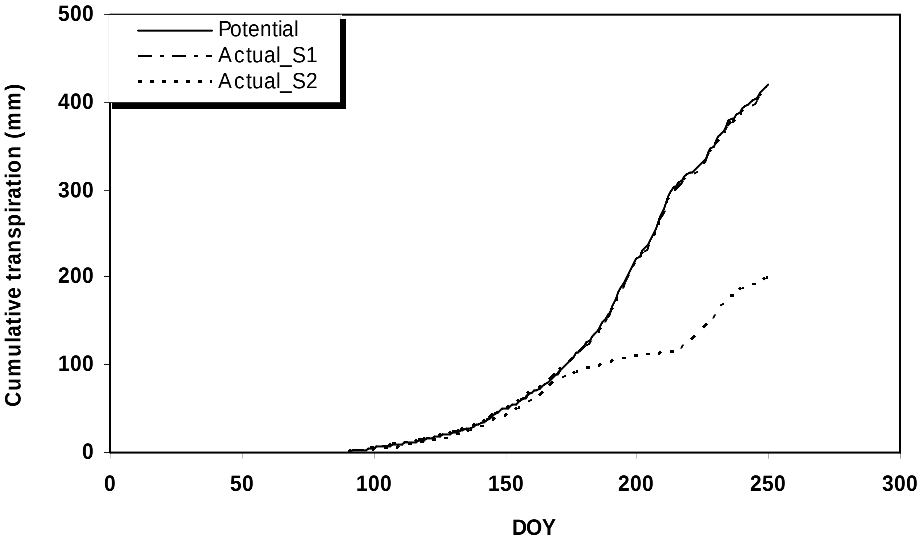
Fig. 8


Potential
Actual_S1
Actual_S2
Cumulative transpiration (mm)
0
100
200
300
400
500
0
50
100
150
200
250
300
DOY

(a)

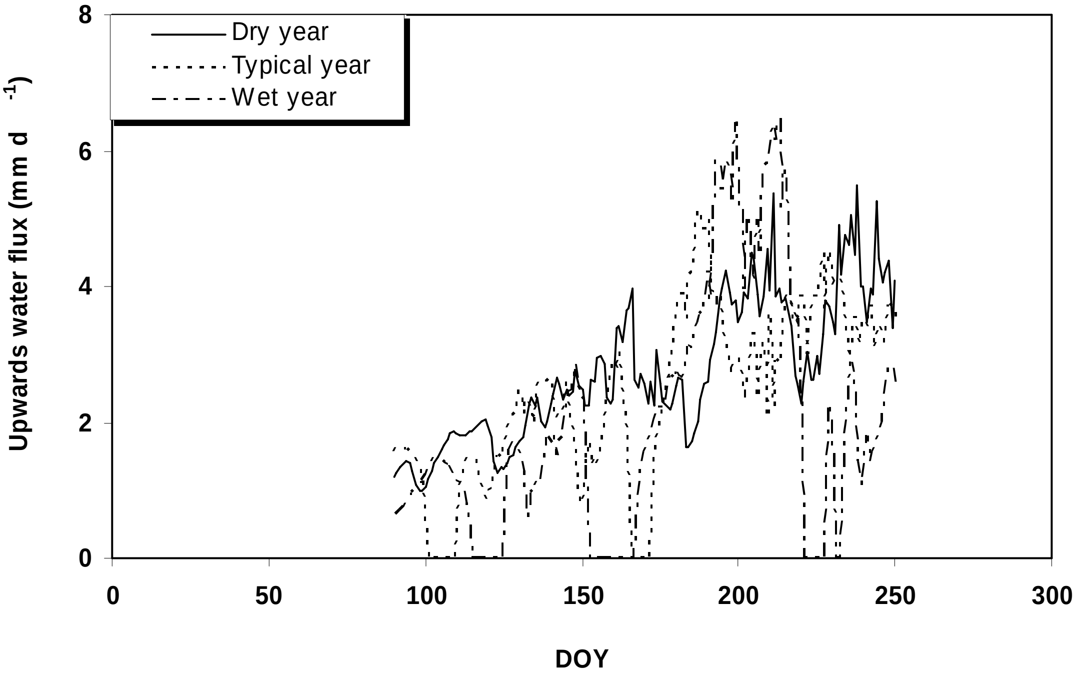

Potential
Actual_S1
Actual_S2
Cumulative transpiration (mm)
0
100
200
300
400
500
0
50
100
150
200
250
300
DOY

(b)


Potential
Actual_S1
Actual_S2
Cumulative transpiration (mm)
0
100
200
300
400
500
0
50
100
150
200
250
300
DOY

(c)

Fig. 9



Dry year
Typical year
Wet year
Upwards water flux (mm d^{-1})
DOY
0
2
4
6
8
0
50
100
150
200
250
300

Fig. 10

Table 1: van Genuchten parameter values in Eqs. (2) and (3) for coarse, medium and fine soils (Wösten et al., 1999)

	Coarse soil	Medium soil	Fine soil
θ_s (cm^3 cm^{-3})	0.40	0.44	0.52
θ_r (cm^3 cm^{-3})	0.025	0.01	0.01
α (–)	0.0383	0.0314	0.0367
n (–)	1.1377	1.1804	1.1012
K_s (cm d^{-1})	60.0	12.1	24.8

Table 2: Summary of the Bouwing and the PAGV experiments

	The Bouwing	The PAGV
Soil type	Silty clay loam	Silty loam
Crop	Wheat	
Sowing date	21 October, 1983	
Harvest date	21 August, 1984	
Measured maximum rooting depth (m)	1.0	
Depths of measured soil water content (cm)	0-20, 20-40, 40-60, 60-80, 80-100	
Dates of soil water measurements (mmdd, 1984)	0214,0313,0403,0424,0508,0528,0619,0703,0717,0807	
Dates of root length measurements (mmdd, 1984)	0425, 0528, 0703	

Table 3: Monthly average rainfall and mean air temperature in the application case

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Rainfall (mm)	52.0	40.4	38.5	50.2	50.2	47.8	57.5	47.3	54.3	64.8	52.9	56.2
Temperature (^oC)	4.8	5.0	7.0	8.9	12.1	15.0	17.3	17.3	14.6	11.0	7.0	4.8

Table 4: Measured particle size distribution and soil organic matter, and soil hydraulic properties derived using PTFs proposed by Wösten et al. (1999) for the topsoil (0 – 45 cm) and subsoil (45 – 100 cm) in the application case

	Topsoil (0 – 45 cm)	Subsoil (45 – 100 cm)
<2 μm (% w w^{-1})	16.0	9.0
2 – 50 μm (% w w^{-1})	22.0	19.0
>50 μm (% w w^{-1})	62.0	72.0
Organic matter (% w w^{-1})	13.4	2.5
θ_s (cm^3 cm^{-3})	0.412	0.425
θ_r (cm^3 cm^{-3})	0.025	0.025
α (–)	0.0138	0.0602
n (–)	1.1557	1.2806
K_s (cm d^{-1})	4.1	38.0

Table 5: Fitted van Genuchten parameter values in Eq. (12) for the Bouwing and the PAGV experiments using the RETC software (van Genuchten et al., 1991)

	The Bouwing		The PAGV		
	0–40 cm	40–100 cm	0–25 cm	25–40 cm	40–100 cm
θ_s (cm^3 cm^{-3})	0.51	0.49	0.42	0.50	0.53
θ_r (cm^3 cm^{-3})	0.00	0.00	0.04	0.06	0.06
α (–)	0.0266	0.0046	0.0162	0.0096	0.0098
n (–)	1.1841	1.1835	1.299	1.3460	1.3193
K_s (cm d^{-1})	40.0	2.0	160.0	33.0	200.0

Table 6: Statistical comparisons between measurement and simulation of relative root length distribution and soil water content in various layers for both the Bouwing and the PAGV experiments

	R^{2*}	RMSE**	ME***
Relative root length distribution	0.855	0.1258	0.0016
Soil water content in layers (cm^3 cm^{-3})	0.801	0.0412	0.0260

*R^2: the coefficient of determination
**RMSE: the root of the mean squared errors
***ME: the mean error